Substitution of Benzylic Hydroxyl Groups with Vinyl Moieties Using Vinylboron Dihalides

George W. Kabalka,^{*} Min-Liang Yao, Scott Borella, Zhong-Zhi Wu

Supporting information

General Methods: All reagents were used as received. Column chromatography was performed using silica gel (60 Å, 230–400 mesh, ICN Biomedicals GmbH, Eschwege, Germany). Analytical thin-layer chromatography was performed using 250 µm silica (Analtech, Inc., Newark, DE).

¹H NMR and ¹³C NMR spectra were recorded at 250.13 and 62.89 MHz, respectively. Chemical shifts for ¹H NMR and ¹³C NMR spectra were referenced to TMS and measured with respect to the residual protons in the deuterated solvents. Microanalysis was performed by Atlantic Microlab, Inc. Norcross, Georgia.

Product 3a: ¹H NMR (250 MHz, CDCl₃): δ 7.56–7.59 (m, 2H), 7.17–7.30 (m, 13H), 6.59 (d, *J* = 9.47 Hz, 1H), 5.42 (d, *J* = 9.47 Hz, 1H). ¹³C NMR (CDCl₃): δ 142.9, 137.8, 133.4, 129.5, 128.6, 128.3, 126.6, 50.8. Anal. Calcd for C₂₁H₁₇Cl: C, 82.75; H, 5.62. Found: C, 82.57; H, 5.65.

Product 3b: ¹H NMR (250 MHz, CDCl₃): δ 7.48–7.51 (m, 2H), 7.12–7.34 (m, 12H), 6.55 (d, *J* = 9.47 Hz, 1H), 5.40 (d, *J* = 9.47 Hz, 1H), 2.34 (s, 3H). ¹³C NMR (CDCl₃): δ

^{*}To Whom Correspondence should be addressed. Phone: (865)974-3260; Fax: (865)974-2997

143.1, 138.7, 135.2, 133.5, 129.0, 128.6, 128.3, 126.5, 50.8, 21.1. Anal. Calcd for $C_{22}H_{19}Cl$: C, 82.87; H, 6.01. Found: C, 82.92; H, 6.03.

Product 3c: 1H NMR (250 MHz, $CDCl_3$): δ 7.53–7.54 (m, 2H), 7.13–7.52 (m, 13H), 6.65 (d, $J = 9.41$ Hz, 1H), 5.36 (d, $J = 9.41$ Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 142.7, 139.6, 133.3, 128.6, 128.3, 128.2, 127.7, 126.6, 126.2, 53.6. Anal. Calcd for $C_{21}H_{17}Br$: C, 72.22; H, 4.91. Found: C, 72.59; H, 4.61.

Product 3d: 1H NMR (250 MHz, $CDCl_3$): δ 7.44–7.47 (m, 2H), 7.10–7.34 (m, 12H), 6.62 (d, $J = 9.37$ Hz, 1H), 5.35 (d, $J = 9.37$ Hz, 1H), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 142.8, 138.7, 136.9, 132.4, 128.9, 128.6, 128.3, 127.6, 126.6, 126.3, 53.6, 21.1. Anal. Calcd for $C_{22}H_{19}Br$: C, 72.73; H, 5.27. Found: C, 72.69; H, 6.11.

Product 3e: 1H NMR (250 MHz, $CDCl_3$): δ 7.59–7.62 (m, 2H), 7.31–7.35 (m, 3H), 7.17 (d, $J = 8.61$ Hz, 4H), 6.85 (d, $J = 8.61$ Hz, 4H), 6.54 (d, $J = 9.58$ Hz, 1H), 5.31 (d, $J = 9.58$ Hz, 1H), 3.78 (s, 6H). ^{13}C NMR ($CDCl_3$): δ 158.2, 137.9, 135.4, 130.1, 129.2, 128.6, 128.3, 126.6, 113.4, 55.2, 49.1. Anal. Calcd for $C_{23}H_{21}ClO_2$: C, 75.71; H, 5.80. Found: C, 75.47; H, 5.96.

Product 3f: 1H NMR (250 MHz, $CDCl_3$): δ 7.19–7.37 (m, 3H), 7.17 (d, $J = 8.63$ Hz, 4H), 6.94–6.97 (m, 1H), 6.85 (d, $J = 8.63$ Hz, 4H), 6.58 (d, $J = 9.49$ Hz, 1H), 5.30 (d, $J = 9.49$ Hz, 1H), 3.74 (s, 6H). ^{13}C NMR ($CDCl_3$): δ 164.5, 160.6, 158.3, 140.1, 140.0, 135.0, 131.3, 131.1, 129.8, 129.1, 122.1, 115.5, 115.2, 114.0, 113.5, 55.1, 49.1. Anal. Calcd for $C_{23}H_{20}ClFO_2$: C, 72.15; H, 5.27. Found: C, 72.22; H, 5.36.

Product 3g: 1H NMR (250 MHz, $CDCl_3$): δ 7.44 (d, $J = 8.21$ Hz, 2H), 7.08–7.17 (m, 6H), 6.83 (d, $J = 8.67$ Hz, 4H), 6.55 (d, $J = 9.37$ Hz, 1H), 5.24 (d, $J = 9.37$ Hz, 1H),

3.77 (s, 6H), 2.33 (s, 3H). ^{13}C NMR (CDCl_3): δ 142.9, 137.8, 133.4, 129.5, 128.6, 128.3, 126.6, 50.8. Anal. Calcd for $\text{C}_{24}\text{H}_{23}\text{BrO}_2$: C, 68.09; H, 5.48. Found: C, 67.93; H, 5.45.

Product 3h: ^1H NMR (250 MHz, CDCl_3): δ 7.48 (d, $J = 8.05$, 2H), 7.11–7.19 (m, 6H), 6.93–7.00 (m, 4H), 6.45 (d, $J = 9.37$ Hz, 1H), 5.34 (d, $J = 9.37$ Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (CDCl_3): δ 163.6, 159.7, 138.9, 138.6, 134.9, 133.9, 129.7, 129.6, 129.0, 128.2, 126.5, 115.6, 115.3, 49.3, 21.1. Anal. Calcd for $\text{C}_{22}\text{H}_{17}\text{ClF}_2$: C, 74.47; H, 4.83. Found: C, 74.88; H, 4.99.

Product 3i: ^1H NMR (250 MHz, CDCl_3): δ 7.56–7.60 (m, 2H), 7.13–7.35 (m, 12H), 6.53 (d, $J = 9.40$ Hz, 1H), 5.36 (d, $J = 9.40$ Hz, 1H). ^{13}C NMR (CDCl_3): δ 142.5, 141.4, 137.7, 133.9, 132.4, 129.6, 128.9, 129.8, 128.7, 128.3, 128.2, 126.8, 126.6, 50.2. Anal. Calcd for $\text{C}_{22}\text{H}_{16}\text{Cl}$: C, 74.35; H, 4.75. Found: C, 74.39; H, 4.87.

Product 3j: ^1H NMR (250 MHz, CDCl_3): δ 7.49 (d, $J = 8.22$ Hz, 2H), 7.11–7.30 (m, 11H), 6.51 (d, $J = 9.23$ Hz, 1H), 5.55 (d, $J = 9.23$ Hz, 1H), 2.34 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (CDCl_3): δ 143.0, 141.3, 138.7, 136.7, 135.1, 133.3, 130.7, 129.0, 128.8, 128.5, 128.1, 126.6, 126.5, 126.4, 126.2, 47.5, 21.1, 19.9. Anal. Calcd for $\text{C}_{23}\text{H}_{21}\text{Cl}$: C, 82.99; H, 6.36. Found: C, 83.28; H, 6.49.

Product 3k: ^1H NMR (250 MHz, CDCl_3): δ 8.14–8.17 (m, 2H), 7.93–7.97 (m, 1H), 7.29–7.62 (m, 11H), 6.26 (d, $J = 9.57$ Hz, 1H), 2.60 (s, 3H). ^{13}C NMR (CDCl_3): δ 147.9, 147.2, 139.5, 133.0, 129.3, 128.8, 128.6, 128.5, 128.2, 123.7, 52.9, 26.0. Anal. Calcd for $\text{C}_{17}\text{H}_{24}\text{O}_2\text{S}$: C, 69.82; H, 8.27. Found: C, 69.83; H, 8.28.

Product 3l: ^1H NMR (250 MHz, CDCl_3): δ 7.46–7.51 (m, 2H), 7.16–7.40 (m, 8H), 6.28 (d, J = 9.02 Hz, 1H), 4.10 (dq, J = 9.02; 7.06 Hz, 1H), 1.45 (d, J = 7.06 Hz, 3H). ^{13}C NMR (CDCl_3): δ 144.4, 139.7, 136.0, 128.5, 128.4, 128.1, 127.6, 127.0, 126.4, 124.2, 42.5, 20.6. Anal. Calcd for $\text{C}_{16}\text{H}_{15}\text{Br}$: C, 66.91; H, 5.26. Found: C, 66.79; H, 5.35.

Product 3m: ^1H NMR (250 MHz, CDCl_3): δ 7.08–7.45 (m, 8H), 6.14 (d, J = 9.02 Hz, 1H), 4.11 (dq, J = 9.02; 6.97 Hz, 1H), 2.42 (s, 3H), 2.30 (s, 3H), 1.42 (d, J = 6.97 Hz, 3H). ^{13}C NMR (CDCl_3): δ 141.9, 138.3, 136.0, 135.1, 131.9, 131.2, 128.9, 127.5, 127.1, 126.3, 39.1, 21.0, 20.8, 16.1. Anal. Calcd for $\text{C}_{18}\text{H}_{19}\text{ClS}$: C, 71.38; H, 6.32. Found: C, 71.81; H, 6.18.

Product 3n: ^1H NMR (250 MHz, CDCl_3): δ 6.85–7.58 (m, 9H), 6.38 (d, J = 8.99 Hz, 1H), 4.41 (dq, J = 8.99; 7.01 Hz, 1H), 3.83 (s, 3H), 1.46 (d, J = 7.01 Hz, 3H). ^{13}C NMR (CDCl_3): δ 157.2, 138.4, 133.2, 132.1, 131.5, 128.2, 127.6, 127.3, 126.5, 120.6, 110.9, 55.4, 35.0, 20.2. Anal. Calcd for $\text{C}_{17}\text{H}_{17}\text{ClO}$: C, 74.86; H, 6.28. Found: C, 75.14; H, 6.21.

Product 3o: ^1H NMR (250 MHz, CDCl_3): δ 8.61–8.72 (m, 2H), 7.22–7.87 (m, 12H), 6.38 (d, J = 9.17 Hz, 1H), 4.44 (dq, J = 9.17; 6.94 Hz, 1H), 1.63 (d, J = 6.94 Hz, 3H). ^{13}C NMR (CDCl_3): δ 143.1, 138.1, 132.4, 132.2, 132.1, 130.7, 130.4, 130.2, 128.9, 128.6, 128.5, 128.3, 126.6, 126.1, 122.6, 120.6, 40.3, 21.1. Anal. Calcd for $\text{C}_{24}\text{H}_{19}\text{Cl}$: C, 84.07; H, 5.59. Found: C, 84.13; H, 5.32.

Product 3p: ^1H NMR (250 MHz, CDCl_3): δ 8.60–8.70 (m, 2H), 7.08–7.85 (m, 11H), 6.32 (d, J = 8.98 Hz, 1H), 4.42 (dq, J = 8.98; 6.95 Hz, 1H), 2.30 (s, 3H), 1.60 (d, J =

6.95 Hz, 3H). ^{13}C NMR (CDCl_3): δ 143.2, 138.4, 132.2, 132.1, 130.7, 130.4, 130.2, 128.9, 128.8, 128.6, 126.6, 126.4, 126.1, 122.6, 120.5, 40.3, 21.1. Anal. Calcd for $\text{C}_{25}\text{H}_{21}\text{Cl}$: C, 84.14; H, 5.93. Found: C, 84.28; H, 6.16.

Product 5: ^1H NMR (250 MHz, CDCl_3): δ 7.20-7.36 (m, 5H), 6.43-6.50 (m, 1H), 6.14-6.23 (m, 1H), 3.56-3.61 (m, 2H), 2.60-2.69 (m, 2H). ^{13}C NMR (CDCl_3): δ 137.0, 132.7, 128.5, 127.3, 126.1, 125.7, 43.9, 36.1.

X-Ray Data for Compound 3b

```
_audit_creation_method      SHELXL-97
_chemical_name_systematic
;
?
;
_chemical_name_common       ?
_chemical_melting_point     ?
_chemical_formula_moiety    ?
_chemical_formula_sum
'C22 H19 Cl'
_chemical_formula_weight    318.82

loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
'C' 'C'  0.0033  0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'H' 'H'  0.0000  0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Cl' 'Cl'  0.1484  0.1585
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting      ?
```

```

_symmetry_space_group_name_H-M    ?

loop_
  _symmetry_equiv_pos_as_xyz
    'x, y, z'
    '-x, y+1/2, -z'

_cell_length_a                     9.871(4)
_cell_length_b                     10.243(4)
_cell_length_c                     16.997(7)
_cell_angle_alpha                   90.00
_cell_angle_beta                   90.397(7)
_cell_angle_gamma                   90.00
_cell_volume                       1718.5(13)
_cell_formula_units_Z               4
_cell_measurement_temperature       173(2)
_cell_measurement_reflns_used       ?
_cell_measurement_theta_min         ?
_cell_measurement_theta_max         ?

_exptl_crystal_description          ?
_exptl_crystal_colour               ?
_exptl_crystal_size_max             ?
_exptl_crystal_size_mid             ?
_exptl_crystal_size_min             ?
_exptl_crystal_density_meas         ?
_exptl_crystal_density_diffrn       1.232
_exptl_crystal_density_method       'not measured'
_exptl_crystal_F_000                672
_exptl_absorpt_coefficient_mu        0.219
_exptl_absorpt_correction_type       ?
_exptl_absorpt_correction_T_min     ?
_exptl_absorpt_correction_T_max     ?
_exptl_absorpt_process_details       ?

_exptl_special_details
;
?
;

_diffrn_ambient_temperature          173(2)
_diffrn_radiation_wavelength          0.71073
_diffrn_radiation_type                MoK\alpha
_diffrn_radiation_source              'fine-focus sealed tube'

```

```

_diffrn_radiation_monochromator  graphite
_diffrn_measurement_device_type  ?
_diffrn_measurement_method      ?
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number        ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%       ?
_diffrn_reflns_number           16168
_diffrn_reflns_av_R_equivalents 0.0693
_diffrn_reflns_av_sigmaI/netI   0.0892
_diffrn_reflns_limit_h_min      -12
_diffrn_reflns_limit_h_max      12
_diffrn_reflns_limit_k_min      -12
_diffrn_reflns_limit_k_max      12
_diffrn_reflns_limit_l_min      -21
_diffrn_reflns_limit_l_max      21
_diffrn_reflns_theta_min        1.20
_diffrn_reflns_theta_max        26.31
_reflns_number_total            6864
_reflns_number_gt               5864
_reflns_threshold_expression     >2sigma(I)

```

```

_computing_data_collection      ?
_computing_cell_refinement      ?
_computing_data_reduction       ?
_computing_structure_solution   'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics   ?
_computing_publication_material ?

```

```
_refine_special_details
```

```
;
```

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is

not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-

factors based on ALL data will be even larger.

```
;
```

```

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type          full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0584P)^2^+0.0511P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details
'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack    0.05(5)
_refine_ls_number_reflns          6864
_refine_ls_number_parameters      417
_refine_ls_number_restraints      1
_refine_ls_R_factor_all           0.0613
_refine_ls_R_factor_gt            0.0501
_refine_ls_wR_factor_ref          0.1313
_refine_ls_wR_factor_gt           0.1207
_refine_ls_goodness_of_fit_ref    1.029
_refine_ls_restrained_S_all       1.028
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_symmetry_multiplicity
  _atom_site_calc_flag
  _atom_site_refinement_flags
  _atom_site_disorder_assembly
  _atom_site_disorder_group
C1 C 0.7491(3) 0.5114(3) -0.09335(17) 0.0411(7) Uani 1 1 d . . .
H1 H 0.6608 0.5147 -0.0715 0.049 Uiso 1 1 calc R . .
C2 C 0.7655(3) 0.4851(3) -0.17343(18) 0.0456(8) Uani 1 1 d . . .

```


H2 H 0.6881 0.4724 -0.2061 0.055 Uiso 1 1 calc R . .
C3 C 0.8913(3) 0.4775(3) -0.20486(16) 0.0367(7) Uani 1 1 d . . .
H3 H 0.9020 0.4596 -0.2593 0.044 Uiso 1 1 calc R . .
C4 C 1.0026(3) 0.4958(3) -0.15777(15) 0.0340(6) Uani 1 1 d . . .
H4 H 1.0907 0.4883 -0.1795 0.041 Uiso 1 1 calc R . .
C5 C 0.9880(3) 0.5253(3) -0.07858(14) 0.0286(6) Uani 1 1 d . . .
H5 H 1.0660 0.5404 -0.0468 0.034 Uiso 1 1 calc R . .
C6 C 0.8617(3) 0.5326(2) -0.04590(15) 0.0280(5) Uani 1 1 d . . .
C7 C 0.8405(3) 0.5647(2) 0.04140(15) 0.0284(5) Uani 1 1 d . . .
H7 H 0.7669 0.5065 0.0613 0.034 Uiso 1 1 calc R . .
C8 C 0.9677(3) 0.5365(3) 0.08975(14) 0.0319(6) Uani 1 1 d . . .
C9 C 0.9943(3) 0.4078(3) 0.11176(16) 0.0362(6) Uani 1 1 d . . .
H9 H 0.9306 0.3413 0.0993 0.043 Uiso 1 1 calc R . .
C10 C 1.1126(3) 0.3758(3) 0.15163(17) 0.0456(8) Uani 1 1 d . . .
H10 H 1.1297 0.2878 0.1663 0.055 Uiso 1 1 calc R . .
C11 C 1.2053(3) 0.4715(3) 0.16996(17) 0.0449(8) Uani 1 1 d . . .
H11 H 1.2865 0.4497 0.1972 0.054 Uiso 1 1 calc R . .
C12 C 1.1801(3) 0.5993(3) 0.14873(17) 0.0417(7) Uani 1 1 d . . .
H12 H 1.2443 0.6654 0.1611 0.050 Uiso 1 1 calc R . .
C13 C 1.0615(3) 0.6311(3) 0.10951(15) 0.0382(6) Uani 1 1 d . . .
H13 H 1.0442 0.7195 0.0959 0.046 Uiso 1 1 calc R . .
C14 C 0.7933(3) 0.7035(2) 0.05044(15) 0.0288(6) Uani 1 1 d . . .
H14 H 0.8430 0.7680 0.0227 0.035 Uiso 1 1 calc R . .
C15 C 0.6896(2) 0.7458(2) 0.09294(14) 0.0249(5) Uani 1 1 d . . .
C16 C 0.6503(2) 0.8838(2) 0.10208(14) 0.0248(5) Uani 1 1 d . . .
C17 C 0.6584(3) 0.9696(3) 0.03873(15) 0.0305(6) Uani 1 1 d . . .
H17 H 0.6840 0.9378 -0.0115 0.037 Uiso 1 1 calc R . .
C18 C 0.6295(3) 1.1003(3) 0.04838(18) 0.0359(6) Uani 1 1 d . . .
H18 H 0.6355 1.1569 0.0043 0.043 Uiso 1 1 calc R . .
C19 C 0.5920(3) 1.1515(3) 0.12071(18) 0.0374(7) Uani 1 1 d . . .
C20 C 0.5827(3) 1.0649(3) 0.18374(17) 0.0343(6) Uani 1 1 d . . .
H20 H 0.5567 1.0967 0.2339 0.041 Uiso 1 1 calc R . .
C21 C 0.6109(3) 0.9335(3) 0.17452(16) 0.0295(6) Uani 1 1 d . . .
H21 H 0.6031 0.8764 0.2183 0.035 Uiso 1 1 calc R . .
C22 C 0.5596(4) 1.2934(3) 0.1310(2) 0.0643(11) Uani 1 1 d . . .
H22A H 0.6316 1.3354 0.1619 0.096 Uiso 1 1 calc R . .
H22B H 0.4732 1.3024 0.1585 0.096 Uiso 1 1 calc R . .
H22C H 0.5528 1.3353 0.0793 0.096 Uiso 1 1 calc R . .
C23 C 0.1300(3) 0.8720(3) 0.59554(15) 0.0310(6) Uani 1 1 d . . .
H23 H 0.1196 0.9598 0.5786 0.037 Uiso 1 1 calc R . .
C24 C 0.1288(3) 0.8436(3) 0.67540(16) 0.0365(6) Uani 1 1 d . . .
H24 H 0.1163 0.9117 0.7125 0.044 Uiso 1 1 calc R . .
C25 C 0.1459(3) 0.7170(3) 0.70109(18) 0.0391(7) Uani 1 1 d . . .
H25 H 0.1461 0.6978 0.7558 0.047 Uiso 1 1 calc R . .

C26 C 0.1627(3) 0.6176(3) 0.64624(17) 0.0370(7) Uani 1 1 d . . .
 H26 H 0.1744 0.5299 0.6633 0.044 Uiso 1 1 calc R . .
 C27 C 0.1623(3) 0.6469(3) 0.56664(15) 0.0320(6) Uani 1 1 d . . .
 H27 H 0.1732 0.5786 0.5294 0.038 Uiso 1 1 calc R . .
 C28 C 0.1461(2) 0.7741(2) 0.54040(14) 0.0260(5) Uani 1 1 d . . .
 C29 C 0.1465(2) 0.8000(2) 0.45133(14) 0.0253(5) Uani 1 1 d . . .
 H29 H 0.2160 0.7415 0.4273 0.030 Uiso 1 1 calc R . .
 C30 C 0.0095(2) 0.7673(2) 0.41358(14) 0.0251(5) Uani 1 1 d . . .
 C31 C -0.1098(3) 0.7856(3) 0.45305(15) 0.0298(6) Uani 1 1 d . . .
 H31 H -0.1074 0.8163 0.5058 0.036 Uiso 1 1 calc R . .
 C32 C -0.2331(3) 0.7603(3) 0.41756(16) 0.0372(7) Uani 1 1 d . . .
 H32 H -0.3148 0.7721 0.4459 0.045 Uiso 1 1 calc R . .
 C33 C -0.2369(3) 0.7174(3) 0.33998(17) 0.0396(7) Uani 1 1 d . . .
 H33 H -0.3214 0.7001 0.3150 0.047 Uiso 1 1 calc R . .
 C34 C -0.1182(3) 0.6999(3) 0.29935(17) 0.0395(7) Uani 1 1 d . . .
 H34 H -0.1209 0.6712 0.2462 0.047 Uiso 1 1 calc R . .
 C35 C 0.0050(3) 0.7239(3) 0.33582(16) 0.0337(6) Uani 1 1 d . . .
 H35 H 0.0868 0.7108 0.3078 0.040 Uiso 1 1 calc R . .
 C36 C 0.1845(2) 0.9383(2) 0.43247(14) 0.0255(5) Uani 1 1 d . . .
 H36 H 0.1190 1.0033 0.4441 0.031 Uiso 1 1 calc R . .
 C37 C 0.2995(2) 0.9795(2) 0.40132(14) 0.0257(5) Uani 1 1 d . . .
 C38 C 0.3339(2) 1.1175(2) 0.38592(13) 0.0256(5) Uani 1 1 d . . .
 C39 C 0.4647(3) 1.1638(3) 0.39865(17) 0.0362(6) Uani 1 1 d . . .
 H39 H 0.5346 1.1048 0.4134 0.043 Uiso 1 1 calc R . .
 C40 C 0.4939(3) 1.2948(3) 0.39003(17) 0.0407(7) Uani 1 1 d . . .
 H40 H 0.5839 1.3245 0.3988 0.049 Uiso 1 1 calc R . .
 C41 C 0.3939(3) 1.3839(3) 0.36879(17) 0.0359(7) Uani 1 1 d . . .
 C42 C 0.2645(3) 1.3371(3) 0.35541(15) 0.0295(6) Uani 1 1 d . . .
 H42 H 0.1946 1.3962 0.3406 0.035 Uiso 1 1 calc R . .
 C43 C 0.2348(3) 1.2059(2) 0.36313(14) 0.0270(5) Uani 1 1 d . . .
 H43 H 0.1453 1.1759 0.3527 0.032 Uiso 1 1 calc R . .
 C44 C 0.4261(4) 1.5271(3) 0.3604(2) 0.0598(10) Uani 1 1 d . . .
 H44A H 0.4394 1.5656 0.4127 0.090 Uiso 1 1 calc R . .
 H44B H 0.3508 1.5712 0.3335 0.090 Uiso 1 1 calc R . .
 H44C H 0.5089 1.5375 0.3296 0.090 Uiso 1 1 calc R . .
 Cl1 Cl 0.59230(7) 0.63493(6) 0.14683(4) 0.03687(18) Uani 1 1 d . . .
 Cl2 Cl 0.42542(7) 0.86761(7) 0.37724(6) 0.0513(2) Uani 1 1 d . . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23

_atom_site_aniso_U_13

_atom_site_aniso_U_12

C1	0.0293(15)	0.0573(19)	0.0369(16)	-0.0054(14)	0.0045(12)	0.0074(13)
C2	0.0424(18)	0.056(2)	0.0386(16)	-0.0097(14)	-0.0122(14)	0.0025(15)
C3	0.0463(18)	0.0376(15)	0.0263(13)	-0.0021(12)	-0.0022(12)	0.0072(13)
C4	0.0378(16)	0.0380(15)	0.0263(13)	0.0059(11)	0.0078(11)	0.0074(12)
C5	0.0278(14)	0.0328(13)	0.0254(12)	-0.0002(11)	0.0016(10)	0.0042(11)
C6	0.0330(14)	0.0214(12)	0.0297(13)	-0.0001(10)	0.0031(10)	0.0009(10)
C7	0.0312(13)	0.0243(13)	0.0297(13)	0.0004(10)	0.0073(10)	0.0013(10)
C8	0.0434(16)	0.0335(14)	0.0188(12)	-0.0019(11)	0.0083(11)	0.0092(12)
C9	0.0498(17)	0.0331(15)	0.0258(14)	0.0035(11)	0.0079(12)	0.0059(13)
C10	0.061(2)	0.0464(19)	0.0299(16)	0.0082(14)	0.0058(14)	0.0184(16)
C11	0.0452(18)	0.066(2)	0.0239(14)	0.0005(14)	0.0004(12)	0.0197(16)
C12	0.0445(17)	0.0503(18)	0.0303(15)	-0.0094(13)	0.0001(12)	0.0054(14)
C13	0.0469(17)	0.0367(15)	0.0309(14)	-0.0044(13)	0.0028(12)	0.0073(14)
C14	0.0341(14)	0.0250(13)	0.0273(13)	0.0008(10)	0.0062(11)	0.0008(10)
C15	0.0274(13)	0.0266(13)	0.0208(12)	-0.0008(10)	0.0003(9)	-0.0024(10)
C16	0.0215(12)	0.0273(13)	0.0255(12)	-0.0035(10)	-0.0014(9)	0.0007(10)
C17	0.0325(14)	0.0328(14)	0.0260(13)	0.0003(11)	0.0027(11)	0.0015(11)
C18	0.0311(15)	0.0313(14)	0.0452(17)	0.0083(12)	0.0023(12)	0.0015(11)
C19	0.0325(14)	0.0287(15)	0.0511(17)	-0.0056(13)	0.0008(12)	0.0027(12)
C20	0.0330(14)	0.0342(15)	0.0357(15)	-0.0088(12)	0.0010(12)	0.0035(12)
C21	0.0294(14)	0.0325(14)	0.0266(13)	-0.0045(11)	-0.0002(10)	0.0027(11)
C22	0.070(3)	0.0309(17)	0.092(3)	-0.0060(18)	0.012(2)	0.0121(17)
C23	0.0347(14)	0.0294(14)	0.0288(14)	0.0025(11)	-0.0006(11)	-0.0013(11)
C24	0.0418(16)	0.0391(15)	0.0287(14)	-0.0018(12)	0.0005(12)	-0.0012(13)
C25	0.0356(15)	0.0499(17)	0.0317(15)	0.0078(13)	-0.0027(12)	-0.0054(13)
C26	0.0352(15)	0.0339(15)	0.0418(16)	0.0130(13)	-0.0050(12)	-0.0001(12)
C27	0.0304(13)	0.0303(14)	0.0353(14)	0.0029(12)	-0.0025(11)	-0.0021(11)
C28	0.0200(12)	0.0297(12)	0.0283(13)	0.0051(10)	0.0009(9)	-0.0022(10)
C29	0.0265(13)	0.0238(12)	0.0258(12)	0.0009(10)	0.0051(10)	-0.0006(10)
C30	0.0300(13)	0.0224(12)	0.0229(12)	0.0025(10)	0.0020(9)	-0.0009(10)
C31	0.0314(14)	0.0362(14)	0.0216(13)	0.0020(11)	0.0011(10)	0.0011(11)
C32	0.0307(14)	0.0487(18)	0.0323(15)	0.0101(13)	0.0006(11)	0.0007(13)
C33	0.0426(17)	0.0419(16)	0.0341(15)	0.0117(12)	-0.0115(13)	-0.0126(13)
C34	0.0560(19)	0.0400(17)	0.0226(13)	0.0011(11)	-0.0021(13)	-0.0108(14)
C35	0.0407(15)	0.0345(14)	0.0261(14)	0.0009(11)	0.0061(11)	-0.0050(12)
C36	0.0245(13)	0.0265(13)	0.0257(12)	0.0011(10)	0.0029(10)	0.0029(10)
C37	0.0241(13)	0.0301(13)	0.0229(12)	0.0037(10)	-0.0008(10)	0.0030(10)
C38	0.0256(13)	0.0315(14)	0.0198(11)	0.0023(10)	0.0039(9)	-0.0019(10)
C39	0.0275(14)	0.0424(16)	0.0387(15)	0.0069(12)	-0.0009(11)	-0.0031(12)
C40	0.0290(15)	0.0481(18)	0.0450(17)	0.0060(14)	0.0001(12)	-0.0123(13)
C41	0.0435(16)	0.0305(16)	0.0338(15)	-0.0016(12)	0.0092(12)	-0.0085(13)
C42	0.0328(14)	0.0284(13)	0.0272(13)	0.0019(10)	0.0032(10)	0.0009(11)

C43 0.0252(12) 0.0334(14) 0.0224(12) 0.0027(10) 0.0021(10) -0.0039(10)
C44 0.067(2) 0.0362(18) 0.077(3) 0.0004(18) 0.0148(19) -0.0173(17)
C11 0.0437(4) 0.0284(3) 0.0387(4) 0.0001(3) 0.0150(3) -0.0032(3)
C12 0.0358(4) 0.0353(4) 0.0832(6) 0.0136(4) 0.0253(4) 0.0104(3)

_geom_special_details

;

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

;

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

C1 C6 1.386(4) . ?

C1 C2 1.398(4) . ?

C1 H1 0.9500 . ?

C2 C3 1.357(4) . ?

C2 H2 0.9500 . ?

C3 C4 1.367(4) . ?

C3 H3 0.9500 . ?

C4 C5 1.388(4) . ?

C4 H4 0.9500 . ?

C5 C6 1.371(4) . ?

C5 H5 0.9500 . ?

C6 C7 1.536(4) . ?

C7 C14 1.505(3) . ?

C7 C8 1.524(3) . ?

C7 H7 1.0000 . ?

C8 C13 1.380(4) . ?

C8 C9 1.395(4) . ?

C9 C10 1.386(4) . ?

C9 H9 0.9500 . ?

C10 C11 1.375(5) . ?

C10 H10 0.9500 . ?

C11 C12 1.379(5) . ?

C11 H11 0.9500 . ?

C12 C13 1.382(4) . ?
C12 H12 0.9500 . ?
C13 H13 0.9500 . ?
C14 C15 1.329(4) . ?
C14 H14 0.9500 . ?
C15 C16 1.474(4) . ?
C15 C11 1.750(3) . ?
C16 C21 1.390(4) . ?
C16 C17 1.393(4) . ?
C17 C18 1.378(4) . ?
C17 H17 0.9500 . ?
C18 C19 1.389(4) . ?
C18 H18 0.9500 . ?
C19 C20 1.394(4) . ?
C19 C22 1.499(4) . ?
C20 C21 1.384(4) . ?
C20 H20 0.9500 . ?
C21 H21 0.9500 . ?
C22 H22A 0.9800 . ?
C22 H22B 0.9800 . ?
C22 H22C 0.9800 . ?
C23 C28 1.383(4) . ?
C23 C24 1.388(4) . ?
C23 H23 0.9500 . ?
C24 C25 1.378(4) . ?
C24 H24 0.9500 . ?
C25 C26 1.392(4) . ?
C25 H25 0.9500 . ?
C26 C27 1.386(4) . ?
C26 H26 0.9500 . ?
C27 C28 1.386(4) . ?
C27 H27 0.9500 . ?
C28 C29 1.537(3) . ?
C29 C36 1.500(3) . ?
C29 C30 1.529(3) . ?
C29 H29 1.0000 . ?
C30 C31 1.372(4) . ?
C30 C35 1.395(4) . ?
C31 C32 1.380(4) . ?
C31 H31 0.9500 . ?
C32 C33 1.390(4) . ?
C32 H32 0.9500 . ?
C33 C34 1.376(5) . ?
C33 H33 0.9500 . ?

C34 C35 1.383(4) . ?
 C34 H34 0.9500 . ?
 C35 H35 0.9500 . ?
 C36 C37 1.325(3) . ?
 C36 H36 0.9500 . ?
 C37 C38 1.477(4) . ?
 C37 C12 1.742(3) . ?
 C38 C43 1.387(3) . ?
 C38 C39 1.391(4) . ?
 C39 C40 1.380(4) . ?
 C39 H39 0.9500 . ?
 C40 C41 1.390(4) . ?
 C40 H40 0.9500 . ?
 C41 C42 1.382(4) . ?
 C41 C44 1.507(4) . ?
 C42 C43 1.382(4) . ?
 C42 H42 0.9500 . ?
 C43 H43 0.9500 . ?
 C44 H44A 0.9800 . ?
 C44 H44B 0.9800 . ?
 C44 H44C 0.9800 . ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
 C6 C1 C2 119.9(3) . . ?
 C6 C1 H1 120.0 . . ?
 C2 C1 H1 120.0 . . ?
 C3 C2 C1 120.5(3) . . ?
 C3 C2 H2 119.8 . . ?
 C1 C2 H2 119.8 . . ?
 C2 C3 C4 119.7(3) . . ?
 C2 C3 H3 120.2 . . ?
 C4 C3 H3 120.2 . . ?
 C3 C4 C5 120.6(3) . . ?
 C3 C4 H4 119.7 . . ?
 C5 C4 H4 119.7 . . ?
 C6 C5 C4 120.4(2) . . ?
 C6 C5 H5 119.8 . . ?

C4 C5 H5 119.8 . . ?
C5 C6 C1 118.9(2) . . ?
C5 C6 C7 122.3(2) . . ?
C1 C6 C7 118.8(2) . . ?
C14 C7 C8 112.3(2) . . ?
C14 C7 C6 110.2(2) . . ?
C8 C7 C6 111.3(2) . . ?
C14 C7 H7 107.6 . . ?
C8 C7 H7 107.6 . . ?
C6 C7 H7 107.6 . . ?
C13 C8 C9 118.3(3) . . ?
C13 C8 C7 123.2(2) . . ?
C9 C8 C7 118.5(2) . . ?
C10 C9 C8 120.7(3) . . ?
C10 C9 H9 119.6 . . ?
C8 C9 H9 119.6 . . ?
C11 C10 C9 119.9(3) . . ?
C11 C10 H10 120.0 . . ?
C9 C10 H10 120.0 . . ?
C10 C11 C12 119.9(3) . . ?
C10 C11 H11 120.0 . . ?
C12 C11 H11 120.0 . . ?
C11 C12 C13 120.0(3) . . ?
C11 C12 H12 120.0 . . ?
C13 C12 H12 120.0 . . ?
C8 C13 C12 121.1(3) . . ?
C8 C13 H13 119.5 . . ?
C12 C13 H13 119.5 . . ?
C15 C14 C7 127.1(2) . . ?
C15 C14 H14 116.4 . . ?
C7 C14 H14 116.4 . . ?
C14 C15 C16 125.0(2) . . ?
C14 C15 C11 120.0(2) . . ?
C16 C15 C11 114.91(18) . . ?
C21 C16 C17 118.1(2) . . ?
C21 C16 C15 121.3(2) . . ?
C17 C16 C15 120.5(2) . . ?
C18 C17 C16 120.5(3) . . ?
C18 C17 H17 119.7 . . ?
C16 C17 H17 119.7 . . ?
C17 C18 C19 121.9(3) . . ?
C17 C18 H18 119.0 . . ?
C19 C18 H18 119.0 . . ?
C18 C19 C20 117.3(3) . . ?

C18 C19 C22 121.9(3) . . ?
C20 C19 C22 120.8(3) . . ?
C21 C20 C19 121.2(3) . . ?
C21 C20 H20 119.4 . . ?
C19 C20 H20 119.4 . . ?
C20 C21 C16 120.9(3) . . ?
C20 C21 H21 119.5 . . ?
C16 C21 H21 119.5 . . ?
C19 C22 H22A 109.5 . . ?
C19 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
C19 C22 H22C 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?
C28 C23 C24 120.8(3) . . ?
C28 C23 H23 119.6 . . ?
C24 C23 H23 119.6 . . ?
C25 C24 C23 120.4(3) . . ?
C25 C24 H24 119.8 . . ?
C23 C24 H24 119.8 . . ?
C24 C25 C26 119.4(3) . . ?
C24 C25 H25 120.3 . . ?
C26 C25 H25 120.3 . . ?
C27 C26 C25 119.7(3) . . ?
C27 C26 H26 120.1 . . ?
C25 C26 H26 120.1 . . ?
C26 C27 C28 121.2(3) . . ?
C26 C27 H27 119.4 . . ?
C28 C27 H27 119.4 . . ?
C23 C28 C27 118.5(2) . . ?
C23 C28 C29 122.9(2) . . ?
C27 C28 C29 118.6(2) . . ?
C36 C29 C30 109.8(2) . . ?
C36 C29 C28 112.1(2) . . ?
C30 C29 C28 111.5(2) . . ?
C36 C29 H29 107.7 . . ?
C30 C29 H29 107.7 . . ?
C28 C29 H29 107.7 . . ?
C31 C30 C35 119.0(2) . . ?
C31 C30 C29 121.6(2) . . ?
C35 C30 C29 119.3(2) . . ?
C30 C31 C32 121.2(2) . . ?
C30 C31 H31 119.4 . . ?
C32 C31 H31 119.4 . . ?

C31 C32 C33 119.5(3) . . ?
C31 C32 H32 120.3 . . ?
C33 C32 H32 120.3 . . ?
C34 C33 C32 120.0(2) . . ?
C34 C33 H33 120.0 . . ?
C32 C33 H33 120.0 . . ?
C33 C34 C35 120.1(3) . . ?
C33 C34 H34 120.0 . . ?
C35 C34 H34 120.0 . . ?
C34 C35 C30 120.2(3) . . ?
C34 C35 H35 119.9 . . ?
C30 C35 H35 119.9 . . ?
C37 C36 C29 127.1(2) . . ?
C37 C36 H36 116.5 . . ?
C29 C36 H36 116.5 . . ?
C36 C37 C38 125.1(2) . . ?
C36 C37 C12 119.9(2) . . ?
C38 C37 C12 115.01(19) . . ?
C43 C38 C39 118.2(2) . . ?
C43 C38 C37 120.8(2) . . ?
C39 C38 C37 120.9(2) . . ?
C40 C39 C38 120.6(3) . . ?
C40 C39 H39 119.7 . . ?
C38 C39 H39 119.7 . . ?
C39 C40 C41 121.2(3) . . ?
C39 C40 H40 119.4 . . ?
C41 C40 H40 119.4 . . ?
C42 C41 C40 117.9(3) . . ?
C42 C41 C44 121.1(3) . . ?
C40 C41 C44 120.9(3) . . ?
C43 C42 C41 121.2(3) . . ?
C43 C42 H42 119.4 . . ?
C41 C42 H42 119.4 . . ?
C42 C43 C38 120.8(2) . . ?
C42 C43 H43 119.6 . . ?
C38 C43 H43 119.6 . . ?
C41 C44 H44A 109.5 . . ?
C41 C44 H44B 109.5 . . ?
H44A C44 H44B 109.5 . . ?
C41 C44 H44C 109.5 . . ?
H44A C44 H44C 109.5 . . ?
H44B C44 H44C 109.5 . . ?

loop_

```

_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C6 C1 C2 C3 1.3(5) . . . . ?
C1 C2 C3 C4 0.0(5) . . . . ?
C2 C3 C4 C5 -1.6(4) . . . . ?
C3 C4 C5 C6 1.9(4) . . . . ?
C4 C5 C6 C1 -0.6(4) . . . . ?
C4 C5 C6 C7 179.9(2) . . . . ?
C2 C1 C6 C5 -1.0(4) . . . . ?
C2 C1 C6 C7 178.5(3) . . . . ?
C5 C6 C7 C14 104.0(3) . . . . ?
C1 C6 C7 C14 -75.5(3) . . . . ?
C5 C6 C7 C8 -21.2(3) . . . . ?
C1 C6 C7 C8 159.3(3) . . . . ?
C14 C7 C8 C13 -27.4(4) . . . . ?
C6 C7 C8 C13 96.7(3) . . . . ?
C14 C7 C8 C9 156.0(2) . . . . ?
C6 C7 C8 C9 -79.9(3) . . . . ?
C13 C8 C9 C10 -0.7(4) . . . . ?
C7 C8 C9 C10 176.1(2) . . . . ?
C8 C9 C10 C11 0.0(4) . . . . ?
C9 C10 C11 C12 0.1(5) . . . . ?
C10 C11 C12 C13 0.4(5) . . . . ?
C9 C8 C13 C12 1.2(4) . . . . ?
C7 C8 C13 C12 -175.4(3) . . . . ?
C11 C12 C13 C8 -1.1(4) . . . . ?
C8 C7 C14 C15 -103.7(3) . . . . ?
C6 C7 C14 C15 131.6(3) . . . . ?
C7 C14 C15 C16 177.8(2) . . . . ?
C7 C14 C15 C11 0.5(4) . . . . ?
C14 C15 C16 C21 -138.4(3) . . . . ?
C11 C15 C16 C21 38.9(3) . . . . ?
C14 C15 C16 C17 38.3(3) . . . . ?
C11 C15 C16 C17 -144.35(19) . . . . ?
C21 C16 C17 C18 0.8(4) . . . . ?
C15 C16 C17 C18 -176.0(2) . . . . ?

```

C16	C17	C18	C19	0.2(4)	.	.	.	.	?
C17	C18	C19	C20	-0.8(4)	.	.	.	.	?
C17	C18	C19	C22	-179.5(3)	.	.	.	.	?
C18	C19	C20	C21	0.5(4)	.	.	.	.	?
C22	C19	C20	C21	179.2(3)	.	.	.	.	?
C19	C20	C21	C16	0.5(4)	.	.	.	.	?
C17	C16	C21	C20	-1.1(4)	.	.	.	.	?
C15	C16	C21	C20	175.7(2)	.	.	.	.	?
C28	C23	C24	C25	1.0(4)	.	.	.	.	?
C23	C24	C25	C26	-0.7(4)	.	.	.	.	?
C24	C25	C26	C27	0.0(4)	.	.	.	.	?
C25	C26	C27	C28	0.4(4)	.	.	.	.	?
C24	C23	C28	C27	-0.5(4)	.	.	.	.	?
C24	C23	C28	C29	179.3(2)	.	.	.	.	?
C26	C27	C28	C23	-0.1(4)	.	.	.	.	?
C26	C27	C28	C29	-180.0(2)	.	.	.	.	?
C23	C28	C29	C36	23.4(3)	.	.	.	.	?
C27	C28	C29	C36	-156.8(2)	.	.	.	.	?
C23	C28	C29	C30	-100.2(3)	.	.	.	.	?
C27	C28	C29	C30	79.6(3)	.	.	.	.	?
C36	C29	C30	C31	-91.1(3)	.	.	.	.	?
C28	C29	C30	C31	33.8(3)	.	.	.	.	?
C36	C29	C30	C35	85.8(3)	.	.	.	.	?
C28	C29	C30	C35	-149.4(2)	.	.	.	.	?
C35	C30	C31	C32	0.8(4)	.	.	.	.	?
C29	C30	C31	C32	177.7(2)	.	.	.	.	?
C30	C31	C32	C33	-1.0(4)	.	.	.	.	?
C31	C32	C33	C34	0.3(4)	.	.	.	.	?
C32	C33	C34	C35	0.5(4)	.	.	.	.	?
C33	C34	C35	C30	-0.7(4)	.	.	.	.	?
C31	C30	C35	C34	0.0(4)	.	.	.	.	?
C29	C30	C35	C34	-176.9(2)	.	.	.	.	?
C30	C29	C36	C37	-127.3(3)	.	.	.	.	?
C28	C29	C36	C37	108.1(3)	.	.	.	.	?
C29	C36	C37	C38	-178.1(2)	.	.	.	.	?
C29	C36	C37	C12	0.5(4)	.	.	.	.	?
C36	C37	C38	C43	-34.6(4)	.	.	.	.	?
C12	C37	C38	C43	146.8(2)	.	.	.	.	?
C36	C37	C38	C39	141.3(3)	.	.	.	.	?
C12	C37	C38	C39	-37.3(3)	.	.	.	.	?
C43	C38	C39	C40	1.1(4)	.	.	.	.	?
C37	C38	C39	C40	-174.9(3)	.	.	.	.	?
C38	C39	C40	C41	0.2(5)	.	.	.	.	?
C39	C40	C41	C42	-0.9(4)	.	.	.	.	?

C39 C40 C41 C44 179.3(3) ?
C40 C41 C42 C43 0.2(4) ?
C44 C41 C42 C43 -179.9(3) ?
C41 C42 C43 C38 1.1(4) ?
C39 C38 C43 C42 -1.7(4) ?
C37 C38 C43 C42 174.3(2) ?

_diffrn_measured_fraction_theta_max 0.991
_diffrn_reflns_theta_full 26.31
_diffrn_measured_fraction_theta_full 0.991
_refine_diff_density_max 0.334
_refine_diff_density_min -0.340
_refine_diff_density_rms 0.055